

Supporting information

**Synthesis, Structure, and Reactivity of the Base-Stabilized Silanone
Molybdenum Complexes**

Takako Muraoka^a, Keisuke Abe^a, Haruhiko Kimura^a, Youhei Haga^a, Keiji Ueno^{a}, and Yusuke*

Sunada^b

^aDivision of Molecular Science, Graduate School of Science and Technology, Gunma University,
Kiryu 376-8515, Japan.

^bInstitute for Materials Chemistry and Engineering, and Graduate School of Engineering Sciences,
Kyushu University, Kasuga, Fukuoka 816-8580, Japan.

*To whom correspondence should be addressed. Tel & fax: +81-277-30-1260. E-mail:
ueno@gunma-u.ac.jp.

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1. General Experimental Methods. All manipulations were performed using either standard Schlenk tube techniques under nitrogen, vacuum line techniques, or a dry box under nitrogen. $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)(=\text{SiMes}_2)]$ (**1**, $\text{Cp}^* = \eta^5\text{-C}_5\text{Me}_5$, $\text{Mes} = 2,4,6\text{-Me}_3\text{C}_6\text{H}_2$) was prepared according to the published procedure.¹ 4-(Dimethylamino)pyridine (DMAP) and pyridine-*N*-oxide (PNO) were recrystallized from toluene before use. Hexane and toluene were dried by refluxing over sodium benzophenone ketyl followed by distillation under a nitrogen atmosphere before use. C_6D_6 was dried over potassium mirror followed by distillation in vacuo before use.

NMR spectra were recorded on a JEOL JNM-AL300, JNM-AL500, JNM-ECS300, JNM-ECS400, or JNM-ECS600 Fourier transform spectrometer at room temperature. IR spectra were recorded on a JASCO FT/IR-600 Plus spectrometer at room temperature. Elemental analyses were performed by the Center for Material Research by Instrumental Analysis, Gunma University, or Institute for Materials Chemistry and Engineering, Kyushu University.

The X-ray intensity data were collected on a RIGAKU RAXIS-IV Imaging Plate diffractometer or a Rigaku VariMax with Saturn CCD diffractometer using graphite-monochromated Mo $\text{K}\alpha$ radiation at 93, 150, or 175 K. Empirical absorption corrections were applied. The structure was solved by direct and Fourier transform methods using the SHELX-97 systems.² All non-hydrogen atoms were refined by full-matrix least-squares techniques with anisotropic displacement parameters based on F^2 with all reflections. All hydrogen atoms except for **2b**·toluene were placed at their geometrically calculated positions and refined riding on the corresponding carbon atoms with isotropic thermal parameters.

2. Synthetic Procedures

2.1 Synthesis of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)\{\text{O}=\text{SiMes}_2(\text{DMAP})\}]$ (2a**).** To a toluene solution (5 mL) of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)(=\text{SiMes}_2)]$ (**1**, 60 mg, 9.6×10^{-5} mol) and DMAP (13 mg, 1.1×10^{-4} mol) was added 1 eq of PNO (8.4 mg, 8.8×10^{-5} mol) at -30°C . The reaction mixture was stirred at -30°C for 15 min. The solution was concentrated to ca. 1 mL in vacuo. The resulting solution was

diluted with hexane (2 mL) and cooled to -30 °C to afford orange crystals of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)\{\text{O}=\text{SiMe}_2(\text{DMAP})\}]$ (**2a**) in 64% yield (43 mg, 5.6×10^{-5} mol). ^1H NMR (300 MHz, C_6D_6) δ / ppm 8.05-8.03 (m, 2H, DMAP), 6.84 (s, 4H, *m*-H), 5.62-5.60 (m, 2H, DMAP), 2.51 (s, 12H, *o*-Me), 2.13 (s, 6H, *p*-Me), 1.93 (s, 15H, C_5Me_5), 1.74 (s, 6H, DMAP), 0.95 (s, 9H, SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (125.7 MHz, C_6D_6) δ / ppm 251.1 (CO), 155.3 (DMAP), 146.4 (DMAP), 145.3 (Mes), 139.4 (Mes), 134.9 (Mes), 129.9 (Mes), 105.6 (DMAP), 103.6 (C_5Me_5), 38.0 (DMAP), 25.1 (*o*-Me), 21.1 (*p*-Me), 11.6 (C_5Me_5), 7.7 (SiMe_3). $^{29}\text{Si}\{^1\text{H}\}$ NMR (99.3 MHz, C_6D_6) δ / ppm 32.4 (SiMe_3), -22.3 (SiMe_2). IR (KBr) ν_{CO} 1865 (s), 1770 (s) cm^{-1} . Anal. Calcd for **2a** $\text{C}_{40}\text{H}_{56}\text{MoN}_2\text{O}_3\text{Si}_2$: C, 62.80; H, 7.38; N, 3.66. Found: C, 63.06; H, 7.38; N, 3.47.

2.2 Synthesis of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)\{\text{O}=\text{SiMe}_2(\text{PNO})\}]$ (2b**).** To a toluene solution (6 mL) of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)(=\text{SiMe}_2)]$ (**1**, 100 mg, 1.60×10^{-4} mol) was added 2 eq of PNO (30 mg, 3.1×10^{-4} mol) at -30 °C. The reaction mixture was stirred at -30 °C for 15 min. The solution was concentrated to ca. 1 mL in vacuo. The resulting solution was diluted with hexane (15 mL) and cooled to -30 °C to afford dark red crystals of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)\{\text{O}=\text{SiMe}_2(\text{PNO})\}]$ (**2b**) in 64% yield (75 mg, 1.0×10^{-4} mol). ^1H NMR (300 MHz, C_6D_6) δ / ppm 8.39 (m, 2H, PNO), 6.69 (s, 4H, *m*-H), 6.34 (m, 2H, PNO), 6.07 (m, 1H, PNO), 2.75-2.54 (br, 12H, *o*-Me), 2.04 (s, 6H, *p*-Me), 1.88 (s, 15H, C_5Me_5), 0.85 (s, 9H, SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (125.7 MHz, C_6D_6) δ / ppm 221.3 (CO), 158.9 (PNO), 153.7 (Mes), 140.8 (Mes), 138.9 (Mes), 137.8 (PNO), 128.8 (Mes), 124.3 (PNO), 104.2 (C_5Me_5), 24.4 (*o*-Me), 21.0 (*p*-Me), 11.0 (C_5Me_5), 7.4 (SiMe_3). $^{29}\text{Si}\{^1\text{H}\}$ NMR (99.3 MHz, C_6D_6) δ / ppm 32.9 (SiMe_3), -13.9 (SiMe_2). IR (KBr) ν_{CO} 1858 (s), 1764 (s) cm^{-1} . Anal. Calcd for **2b**·0.5toluene $\text{C}_{41.5}\text{H}_{55}\text{MoNO}_4\text{Si}_2$: C, 63.58; H, 7.07; N, 1.79. Found: C, 63.26; H, 6.84; N, 1.85.

2.3 Isolation of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)(\text{DMAP})]$ (3**).** A C_6D_6 (0.5 mL) solution of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)\{\text{O}=\text{SiMe}_2(\text{DMAP})\}]$ (**2a**, 17 mg, 2.3×10^{-5} mol) was allowed to stand at 25 °C for 8 days. Volatiles were removed from the solution in vacuo. The residue was washed with hexane (1 mL $\times$ 3) to give yellow crystals of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)(\text{DMAP})]$ (**3**) in 44% yield (5 mg,

1×10^{-5} mol). ^1H NMR (300 MHz, C_6D_6) δ / ppm 8.19-8.17 (m, 2H, DMAP), 5.48-5.45 (m, 2H, DMAP), 1.96 (s, 6H, DMAP), 1.74 (s, 15H, C_5Me_5), 1.03 (s, 9H, SiMe_3). $^{13}\text{C}\{^1\text{H}\}$ NMR (125.7 MHz, C_6D_6) δ / ppm 247.2 (CO), 158.0 (DMAP), 153.5 (DMAP), 107.5 (DMAP), 102.4 (C_5Me_5), 38.0 (DMAP), 11.0 (C_5Me_5), 7.3 (SiMe_3). $^{29}\text{Si}\{^1\text{H}\}$ NMR (99.3 MHz, C_6D_6) δ / ppm 32.4 (SiMe_3). IR (KBr) $\nu_{\text{C=O}}$ 1878 (s), 1796 (s) cm^{-1} . Anal. Calcd for **3** $\text{C}_{22}\text{H}_{34}\text{MoN}_2\text{O}_2\text{Si}$: C, 54.76; H, 7.10; N, 5.81. Found: C, 54.71; H, 6.88; N, 5.88.

2.4 Isolation of *cis*-[Cp*(OC)₂Mo{OSiMes₂(OSiMe₃)}(PMe₃)] (4). To a toluene solution (25 mL) of [Cp*(OC)₂Mo(SiMe₃){O=SiMes₂(PNO)}] (**2b**, 355 mg, 4.8×10^{-4} mol) was added excess PMe₃ (500 μL , 4.8×10^{-3} mol) at 25 °C. The reaction mixture was stirred at 25 °C for 19 h. Volatiles were removed from the solution in vacuo. The residue was extracted with pentane (3 mL) and the extract was filtered through a glass filter. Evaporation of volatiles from the filtrate in vacuo gave red-brown waxy solids of *cis*-[Cp*(OC)₂Mo{OSiMes₂(OSiMe₃)}(PMe₃)] (**4**) in 75% yield (263 mg, 3.6×10^{-4} mol). ^1H NMR (400 MHz, C_6D_6) δ / ppm 6.84 (s, 2H, *m*-H), 6.82 (s, 2H, *m*-H), 2.56 (s, 6H, *o*-Me), 2.54 (s, 6H, *o*-Me), 2.21 (s, 3H, *p*-Me), 2.18 (s, 3H, *p*-Me), 1.59 (s, 15H, C_5Me_5), 1.13 (d, $^2J_{\text{H-P}} = 12$ Hz, 9H, PMe₃), 0.12 (s, 9H, SiMe₃). $^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, C_6D_6) δ / ppm 270.0 (d, $^2J_{\text{C-P}} = 35$ Hz, CO), 249.3 (d, $^2J_{\text{C-P}} = 13$ Hz, CO), 143.8 (Ar), 143.3 (Ar), 143.0 (Ar), 142.8 (Ar), 140.3 (Ar), 138.9 (Ar), 137.0 (Ar), 136.6 (Ar), 106.3 (C_5Me_5), 25.2 (*o*-Me), 25.1 (*o*-Me), 20.9 (*p*-Me), 20.8 (*p*-Me), 16.0 (d, $^1J_{\text{C-P}} = 24$ Hz, PMe₃), 11.0 (C_5Me_5), 2.8 (SiMe₃). $^{31}\text{P}\{^1\text{H}\}$ NMR (242.9 MHz, C_6D_6) δ / ppm 3.4 (PMe₃). $^{29}\text{Si}\{^1\text{H}\}$ NMR (119.2 MHz, C_6D_6) δ / ppm 3.2 (SiMe₃), -36.5 (SiMes₂). IR (KBr) 1931 (vs, $\nu_{\text{C=O}}$), 1833 (vs, $\nu_{\text{C=O}}$), 1018 (s, $\nu_{\text{Si-O-Si}}$) cm^{-1} . Anal. Calcd for **4** $\text{C}_{36}\text{H}_{55}\text{MoO}_4\text{PSi}_2$: C, 58.84; H, 7.54. Found: C, 59.16; H, 7.65.

3. X-ray crystal structure determination of [Cp*(OC)₂Mo(SiMe₃){O=SiMes₂(DMAP)}·(C₆H₁₄)_{0.5}] (2a·0.5 hexane). A single crystal of **2a**·0.5 hexane suitable for X-ray crystal structure determination was obtained by recrystallization from a THF/hexane solution of **2a**. The final residue *R*1 and the weighted *wR*2 were 0.0420 and 0.0989,

respectively. Crystallographic data, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, and anisotropic displacement parameters are listed in Tables S-1, S-2, S-3, and S-4, respectively. ORTEP drawing of **2a** with atomic numbering schemes is shown in Figure S-1.

X-ray crystal structure determination of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)\{\text{O}=\text{SiMe}_2(\text{PNO})\} \cdot \text{C}_7\text{H}_8]$ (2b**·toluene).** A single crystal of **2b**·toluene suitable for X-ray crystal structure determination was obtained by recrystallization from a toluene/hexane solution of **2b**. The final residue *R*1 and the weighted *wR*2 were 0.1162 and 0.3162, respectively. Crystallographic data, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, and anisotropic displacement parameters are listed in Tables S-5 S-6 S-7 and S-8 respectively. ORTEP drawing of **2b** with atomic numbering schemes is shown in Figure S-2.

X-ray crystal structure determination of $[\text{Cp}^*(\text{OC})_2\text{Mo}(\text{SiMe}_3)(\text{DMAP})]$ (3**).** A single crystal of **3** suitable for X-ray crystal structure determination was obtained by recrystallization from a toluene/hexane solution of **3**. The final residue *R*1 and the weighted *wR*2 were 0.0284 and 0.0743, respectively. Crystallographic data, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, and anisotropic displacement parameters are listed in Tables S-9, S-10, S-11, and S-12, respectively. ORTEP drawing of **3** with atomic numbering schemes is shown in Figure S-3.

Table S-1. Crystal data and structure refinement for complex **2a**·0.5 hexane.

Complex	Cp*(OC) ₂ Mo(SiMe ₃) {O=SiMes ₂ (DMAP)} · (C ₆ H ₁₄) _{0.5} (2a ·0.5 hexane)	
Empirical formula	C ₄₃ H ₆₃ MoN ₂ O ₃ Si ₂	
Formula weight	808.07	
Temperature (K)	93(2)	
Wavelength (Å)	0.71073	
Crystal system	Monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	<i>a</i> = 11.8339(11) Å	
	<i>b</i> = 21.296(2) Å	<i>β</i> = 102.9590(10)°
	<i>c</i> = 17.1916(17) Å	
Volume (Å ³)	4222.2(7)	
<i>Z</i>	4	
<i>D</i> _{calc} (Mg / m ³)	1.271	
Absorption coefficient (mm ⁻¹)	4.058	
<i>F</i> (000)	1716	
Crystal Size (mm ³)	0.060 × 0.060 × 0.040	
<i>θ</i> Range for data collection (°)	3.04 – 27.49	
Index ranges	–15 ≤ <i>h</i> ≤ 15, –27 ≤ <i>k</i> ≤ 27, –20 ≤ <i>l</i> ≤ 22	
Reflections collected	34127	
Independent reflections [<i>R</i> (int)]	9672 [0.0566]	
Absorption correction	Semi-empirical from equivalents	
Maximum and minimum transmission	0.984 and 0.814	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	9672 / 76 / 506	
Goodness-of-fit on <i>F</i> ²	1.050	
Final <i>R</i> indices ^a [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0420, <i>wR</i> 2 = 0.0989	
<i>R</i> indices ^a (all data)	<i>R</i> 1 = 0.0550, <i>wR</i> 2 = 0.1064	
Largest difference in peak and hole (eÅ ⁻³)	0.711 and -0.617	

^a*R*1 = Σ||*F**o*| – |*F**c*|| / Σ|*F**o*|.

*wR*2 = [Σ[*w* (*F**o*² – *F**c*²)²] / Σ[*w* (*F**o*²)²]]^{0.5},

calc *w* = 1 / [σ²(*F**o*²) + (0.0545 *P*)² + 0.0000 *P*] where *P* = (*F**o*² + 2*F**c*²) / 3.

Table S-2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2a**·0.5 hexane. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Mo	2024(1)	6914(1)	1888(1)	196(1)
Si(1)	960(1)	6023(1)	977(1)	264(2)
Si(2)	5014(1)	6920(1)	3059(1)	196(1)
O(1)	3262(1)	6562(1)	531(1)	293(4)
O(2)	1722(2)	5708(1)	2853(1)	359(4)
O(3)	3716(1)	7066(1)	2680(1)	233(3)
N(1)	5420(2)	6261(1)	2450(1)	210(4)
N(2)	5970(2)	4700(1)	1119(1)	272(4)
C(1)	2827(2)	6669(1)	1068(1)	231(5)
C(2)	1887(2)	6149(1)	2482(1)	263(5)
C(3)	499(2)	6209(1)	-124(1)	335(6)
C(4)	-422(2)	5702(1)	1224(2)	418(7)
C(5)	1870(2)	5291(1)	997(2)	312(5)
C(6)	6015(2)	7590(1)	2953(1)	218(5)
C(7)	6663(2)	7927(1)	3611(1)	238(5)
C(8)	7472(2)	8372(1)	3498(1)	267(5)
C(9)	7676(2)	8504(1)	2748(2)	261(5)
C(10)	6972(2)	8212(1)	2099(1)	249(5)
C(11)	6137(2)	7773(1)	2179(1)	228(5)
C(12)	6504(2)	7835(1)	4453(1)	283(5)
C(13)	8631(2)	8945(1)	2637(2)	355(6)
C(14)	5367(2)	7521(1)	1416(1)	289(5)
C(15)	5335(2)	6498(1)	4058(1)	231(5)
C(16)	4459(2)	6391(1)	4490(1)	257(5)
C(17)	4691(2)	5992(1)	5157(1)	289(5)
C(18)	5752(2)	5708(1)	5436(1)	303(6)
C(19)	6616(2)	5837(1)	5038(1)	315(6)
C(20)	6433(2)	6217(1)	4359(1)	273(5)
C(21)	3297(2)	6707(1)	4302(1)	316(6)
C(22)	5945(3)	5290(1)	6159(2)	396(7)
C(23)	7466(2)	6310(1)	3986(2)	353(6)
C(24)	4709(2)	5754(1)	2362(1)	224(5)
C(25)	4873(2)	5230(1)	1949(1)	249(5)
C(26)	5809(2)	5197(1)	1564(1)	226(5)

C(27)	6564(2)	5721(1)	1680(1)	262(5)
C(28)	6350(2)	6223(1)	2114(1)	250(5)
C(29)	5165(2)	4176(1)	995(2)	375(6)
C(30)	6953(2)	4689(1)	740(2)	364(6)
C(31)	1637(2)	7858(2)	2534(1)	297(6)
C(32)	616(2)	7500(1)	2398(1)	287(5)
C(33)	215(2)	7429(1)	1555(1)	289(5)
C(34)	1000(2)	7756(1)	1168(1)	290(5)
C(35)	1893(2)	8008(1)	1777(2)	297(6)
C(36)	2325(3)	8101(1)	3315(2)	429(7)
C(37)	4(2)	7263(1)	3016(2)	415(7)
C(38)	-991(2)	7224(2)	1152(2)	445(7)
C(39)	813(3)	7870(1)	293(2)	402(7)
C(40)	2891(2)	8408(1)	1670(2)	466(7)
C(41A)	10863(7)	5246(3)	6875(4)	69(2)
C(41B)	10840(20)	5029(10)	6839(9)	106(6)
C(42A)	10058(6)	4956(3)	6121(4)	85(2)
C(42B)	10456(16)	5323(6)	5995(9)	99(3)
C(43A)	10429(5)	5158(3)	5391(3)	82(2)
C(43B)	9871(15)	4843(6)	5410(6)	105(3)

Table S-3. Bond lengths [Å] and angles [°] for **2a**·0.5 hexane.

Mo-Si(1)	2.5991(7)	C(10)-C(11)	1.389(3)
Mo-O(3)	2.178(2)	C(11)-C(14)	1.517(3)
Mo-C(1)	1.940(2)	C(15)-C(16)	1.422(3)
Mo-C(2)	1.948(2)	C(15)-C(20)	1.420(3)
Mo-C(31)	2.391(2)	C(16)-C(17)	1.403(3)
Mo-C(32)	2.399(2)	C(16)-C(21)	1.501(3)
Mo-C(33)	2.358(2)	C(17)-C(18)	1.379(4)
Mo-C(34)	2.354(2)	C(18)-C(19)	1.380(4)
Mo-C(35)	2.340(2)	C(18)-C(22)	1.504(3)
Si(1)-C(3)	1.890(3)	C(19)-C(20)	1.397(3)
Si(1)-C(4)	1.906(3)	C(20)-C(23)	1.515(4)
Si(1)-C(5)	1.890(3)	C(24)-C(25)	1.360(3)
Si(2)-O(3)	1.560(2)	C(25)-C(26)	1.414(3)
Si(2)-N(1)	1.876(2)	C(26)-C(27)	1.415(3)
Si(2)-C(15)	1.899(2)	C(27)-C(28)	1.359(3)
Si(2)-C(6)	1.888(2)	C(31)-C(32)	1.403(4)
O(1)-C(1)	1.176(3)	C(31)-C(35)	1.437(3)
O(2)-C(2)	1.176(3)	C(31)-C(36)	1.498(3)
N(1)-C(24)	1.357(3)	C(32)-C(33)	1.429(3)
N(1)-C(28)	1.355(3)	C(32)-C(37)	1.502(3)
N(2)-C(26)	1.345(3)	C(33)-C(34)	1.437(3)
N(2)-C(29)	1.452(3)	C(33)-C(38)	1.504(3)
N(2)-C(30)	1.456(3)	C(34)-C(35)	1.416(4)
C(6)-C(7)	1.412(3)	C(34)-C(39)	1.491(3)
C(6)-C(11)	1.425(3)	C(35)-C(40)	1.501(4)
C(7)-C(8)	1.392(3)	C(41A)-C(42A)	1.553(8)
C(7)-C(12)	1.512(3)	C(41B)-C(42B)	1.551(10)
C(8)-C(9)	1.394(3)	C(42A)-C(43A)	1.483(7)
C(9)-C(10)	1.381(3)	C(42B)-C(43B)	1.491(10)
C(9)-C(13)	1.514(3)		
Si(1)-Mo-O(3)	137.59(4)	Si(1)-Mo-C(31)	140.94(6)
Si(1)-Mo-C(1)	67.41(7)	Si(1)-Mo-C(32)	108.51(6)
Si(1)-Mo-C(2)	67.63(7)	Si(1)-Mo-C(33)	84.39(6)
Si(1)-Mo-C(34)	96.70(7)	O(3)-Si(2)-N(1)	105.50(9)
Si(1)-Mo-C(35)	131.57(7)	O(3)-Si(2)-C(6)	112.92(9)

O(3)-Mo-C(1)	87.87(8)	O(3)-Si(2)-C(15)	116.78(10)
O(3)-Mo-C(2)	88.22(8)	N(1)-Si(2)-C(6)	105.44(9)
O(3)-Mo-C(31)	80.20(7)	N(1)-Si(2)-C(15)	97.30(9)
O(3)-Mo-C(32)	108.10(7)	C(6)-Si(2)-C(15)	116.22(9)
O(3)-Mo-C(33)	137.72(7)	Mo-O(3)-Si(2)	155.91(10)
O(3)-Mo-C(34)	120.55(8)	Si(2)-N(1)-C(24)	115.31(15)
O(3)-Mo-C(35)	86.45(8)	Si(2)-N(1)-C(28)	128.10(15)
C(1)-Mo-C(2)	105.52(10)	C(24)-N(1)-C(28)	116.54(19)
C(1)-Mo-C(31)	137.75(9)	C(26)-N(2)-C(29)	121.1(2)
C(1)-Mo-C(32)	154.03(9)	C(26)-N(2)-C(30)	119.8(2)
C(1)-Mo-C(33)	120.97(9)	C(29)-N(2)-C(30)	118.0(2)
C(1)-Mo-C(34)	95.83(9)	Mo-C(1)-O(1)	174.2(2)
C(1)-Mo-C(35)	104.07(9)	Mo-C(2)-O(2)	174.4(2)
C(2)-Mo-C(31)	114.36(10)	Si(2)-C(6)-C(7)	123.10(17)
C(2)-Mo-C(32)	95.57(9)	Si(2)-C(6)-C(11)	119.59(16)
C(2)-Mo-C(33)	109.77(9)	C(7)-C(6)-C(11)	117.3(2)
C(2)-Mo-C(34)	144.95(9)	C(6)-C(7)-C(8)	120.1(2)
C(2)-Mo-C(35)	149.69(9)	C(6)-C(7)-C(12)	122.6(2)
C(31)-Mo-C(32)	34.07(9)	C(8)-C(7)-C(12)	117.3(2)
C(31)-Mo-C(33)	57.57(8)	C(7)-C(8)-C(9)	122.3(2)
C(31)-Mo-C(34)	58.25(8)	C(8)-C(9)-C(10)	117.2(2)
C(31)-Mo-C(35)	35.35(8)	C(8)-C(9)-C(13)	122.1(2)
C(32)-Mo-C(33)	34.93(8)	C(10)-C(9)-C(13)	120.7(2)
C(32)-Mo-C(34)	58.54(8)	C(9)-C(10)-C(11)	122.5(2)
C(32)-Mo-C(35)	58.22(9)	C(6)-C(11)-C(10)	120.0(2)
C(33)-Mo-C(34)	35.52(8)	C(6)-C(11)-C(14)	123.0(2)
C(33)-Mo-C(35)	58.49(9)	C(10)-C(11)-C(14)	117.0(2)
C(34)-Mo-C(35)	35.11(9)	Si(2)-C(15)-C(16)	121.83(17)
Mo-Si(1)-C(3)	116.22(9)	Si(2)-C(15)-C(20)	120.65(17)
Mo-Si(1)-C(4)	116.89(9)	C(16)-C(15)-C(20)	117.2(2)
Mo-Si(1)-C(5)	113.19(8)	C(15)-C(16)-C(17)	119.5(2)
C(3)-Si(1)-C(4)	103.24(12)	C(15)-C(16)-C(21)	123.7(2)
C(3)-Si(1)-C(5)	103.09(12)	C(17)-C(16)-C(21)	116.7(2)
C(4)-Si(1)-C(5)	102.35(12)	C(16)-C(17)-C(18)	123.1(2)
C(17)-C(18)-C(19)	117.3(2)	C(31)-C(32)-C(33)	107.7(2)
C(17)-C(18)-C(22)	120.3(2)	C(31)-C(32)-C(37)	126.8(2)
C(19)-C(18)-C(22)	122.4(2)	C(33)-C(32)-C(37)	125.4(2)
C(18)-C(19)-C(20)	122.4(2)	Mo-C(33)-C(32)	74.09(13)

C(15)-C(20)-C(19)	120.4(2)	Mo-C(33)-C(34)	72.05(13)
C(15)-C(20)-C(23)	123.4(2)	Mo-C(33)-C(38)	133.86(18)
C(19)-C(20)-C(23)	116.1(2)	C(32)-C(33)-C(34)	108.4(2)
N(1)-C(24)-C(25)	123.7(2)	C(32)-C(33)-C(38)	124.2(2)
C(24)-C(25)-C(26)	120.2(2)	C(34)-C(33)-C(38)	124.9(2)
N(2)-C(26)-C(25)	122.0(2)	Mo-C(34)-C(33)	72.43(13)
N(2)-C(26)-C(27)	122.4(2)	Mo-C(34)-C(35)	71.92(13)
C(25)-C(26)-C(27)	115.6(2)	Mo-C(34)-C(39)	126.64(18)
C(26)-C(27)-C(28)	120.5(2)	C(33)-C(34)-C(35)	107.2(2)
N(1)-C(28)-C(27)	123.4(2)	C(33)-C(34)-C(39)	125.5(2)
Mo-C(31)-C(32)	73.30(14)	C(35)-C(34)-C(39)	127.0(2)
Mo-C(31)-C(35)	70.40(13)	Mo-C(35)-C(31)	74.25(14)
Mo-C(31)-C(36)	125.76(17)	Mo-C(35)-C(34)	72.97(14)
C(32)-C(31)-C(35)	108.6(2)	Mo-C(35)-C(40)	122.36(17)
C(32)-C(31)-C(36)	127.7(2)	C(31)-C(35)-C(34)	108.1(2)
C(35)-C(31)-C(36)	123.6(3)	C(31)-C(35)-C(40)	124.6(2)
Mo-C(32)-C(31)	72.63(13)	C(34)-C(35)-C(40)	127.1(2)
Mo-C(32)-C(33)	70.98(13)	C(41A)-C(42A)-C(43A)	110.4(6)
Mo-C(32)-C(37)	124.65(17)	C(41B)-C(42B)-C(43B)	110.4(9)

Table S-4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2a**·0.5 hexane. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo	19(1)	22(1)	18(1)	-2(1)	5(1)	1(1)
Si(1)	22(1)	32(1)	27(1)	-5(1)	7(1)	-6(1)
Si(2)	21(1)	20(1)	18(1)	-1(1)	5(1)	1(1)
O(1)	30(1)	34(1)	27(1)	-11(1)	14(1)	-8(1)
O(2)	41(1)	33(1)	35(1)	6(1)	11(1)	-3(1)
O(3)	23(1)	26(1)	20(1)	-3(1)	3(1)	0(1)
N(1)	22(1)	21(1)	21(1)	0(1)	8(1)	1(1)
N(2)	30(1)	21(1)	33(1)	-7(1)	13(1)	-1(1)
C(1)	21(1)	22(1)	25(1)	-3(1)	2(1)	-4(1)
C(2)	24(1)	32(1)	24(1)	-3(1)	6(1)	0(1)
C(3)	27(1)	41(2)	31(1)	-8(1)	4(1)	-5(1)
C(4)	30(1)	53(2)	44(2)	-10(1)	12(1)	-16(1)
C(5)	35(1)	29(1)	31(1)	-7(1)	10(1)	-9(1)
C(6)	19(1)	22(1)	24(1)	0(1)	4(1)	2(1)
C(7)	22(1)	24(1)	24(1)	-2(1)	2(1)	7(1)
C(8)	25(1)	23(1)	29(1)	-5(1)	-1(1)	2(1)
C(9)	23(1)	22(1)	33(1)	-1(1)	6(1)	2(1)
C(10)	29(1)	21(1)	25(1)	2(1)	7(1)	3(1)
C(11)	26(1)	20(1)	23(1)	0(1)	6(1)	2(1)
C(12)	33(1)	30(1)	21(1)	-4(1)	2(1)	1(1)
C(13)	34(1)	29(1)	43(2)	-3(1)	8(1)	-6(1)
C(14)	35(1)	29(1)	23(1)	1(1)	6(1)	-6(1)
C(15)	28(1)	23(1)	19(1)	-2(1)	5(1)	0(1)
C(16)	32(1)	25(1)	20(1)	-4(1)	6(1)	-2(1)
C(17)	44(2)	24(1)	21(1)	-3(1)	13(1)	-4(1)
C(18)	47(2)	20(1)	22(1)	-3(1)	3(1)	-1(1)
C(19)	37(1)	26(1)	28(1)	0(1)	0(1)	7(1)
C(20)	32(1)	25(1)	24(1)	-3(1)	5(1)	4(1)
C(21)	35(1)	39(1)	24(1)	-1(1)	13(1)	3(1)
C(22)	63(2)	27(1)	26(1)	3(1)	4(1)	-2(1)
C(23)	26(1)	40(2)	38(2)	4(1)	3(1)	7(1)
C(24)	20(1)	24(1)	25(1)	2(1)	8(1)	1(1)
C(25)	23(1)	22(1)	31(1)	0(1)	7(1)	-1(1)
C(26)	24(1)	20(1)	24(1)	0(1)	6(1)	2(1)

C(27)	27(1)	25(1)	30(1)	-3(1)	15(1)	-1(1)
C(28)	25(1)	22(1)	28(1)	-4(1)	9(1)	-3(1)
C(29)	33(1)	26(1)	54(2)	-14(1)	10(1)	-4(1)
C(30)	51(2)	27(1)	39(2)	-7(1)	25(1)	2(1)
C(31)	36(1)	26(1)	26(1)	-6(1)	3(1)	12(1)
C(32)	31(1)	33(1)	24(1)	1(1)	10(1)	15(1)
C(33)	23(1)	37(1)	27(1)	-4(1)	5(1)	12(1)
C(34)	30(1)	31(1)	26(1)	3(1)	7(1)	12(1)
C(35)	34(1)	21(1)	34(1)	2(1)	9(1)	8(1)
C(36)	50(2)	35(2)	37(2)	-14(1)	-4(1)	15(1)
C(37)	41(2)	54(2)	34(2)	5(1)	18(1)	19(1)
C(38)	22(1)	66(2)	44(2)	-9(2)	3(1)	14(1)
C(39)	45(2)	51(2)	26(1)	9(1)	8(1)	12(1)
C(40)	47(2)	29(2)	65(2)	4(1)	14(2)	2(1)
C(41A)	69(4)	53(4)	102(4)	22(3)	52(3)	16(3)
C(41B)	120(10)	106(11)	94(7)	19(8)	26(8)	6(10)
C(42A)	97(4)	81(4)	90(4)	24(3)	46(3)	20(3)
C(42B)	117(6)	83(6)	95(5)	36(5)	24(6)	11(5)
C(43A)	102(4)	68(4)	85(4)	13(3)	39(3)	28(3)
C(43B)	134(7)	81(6)	94(5)	22(6)	14(6)	40(5)

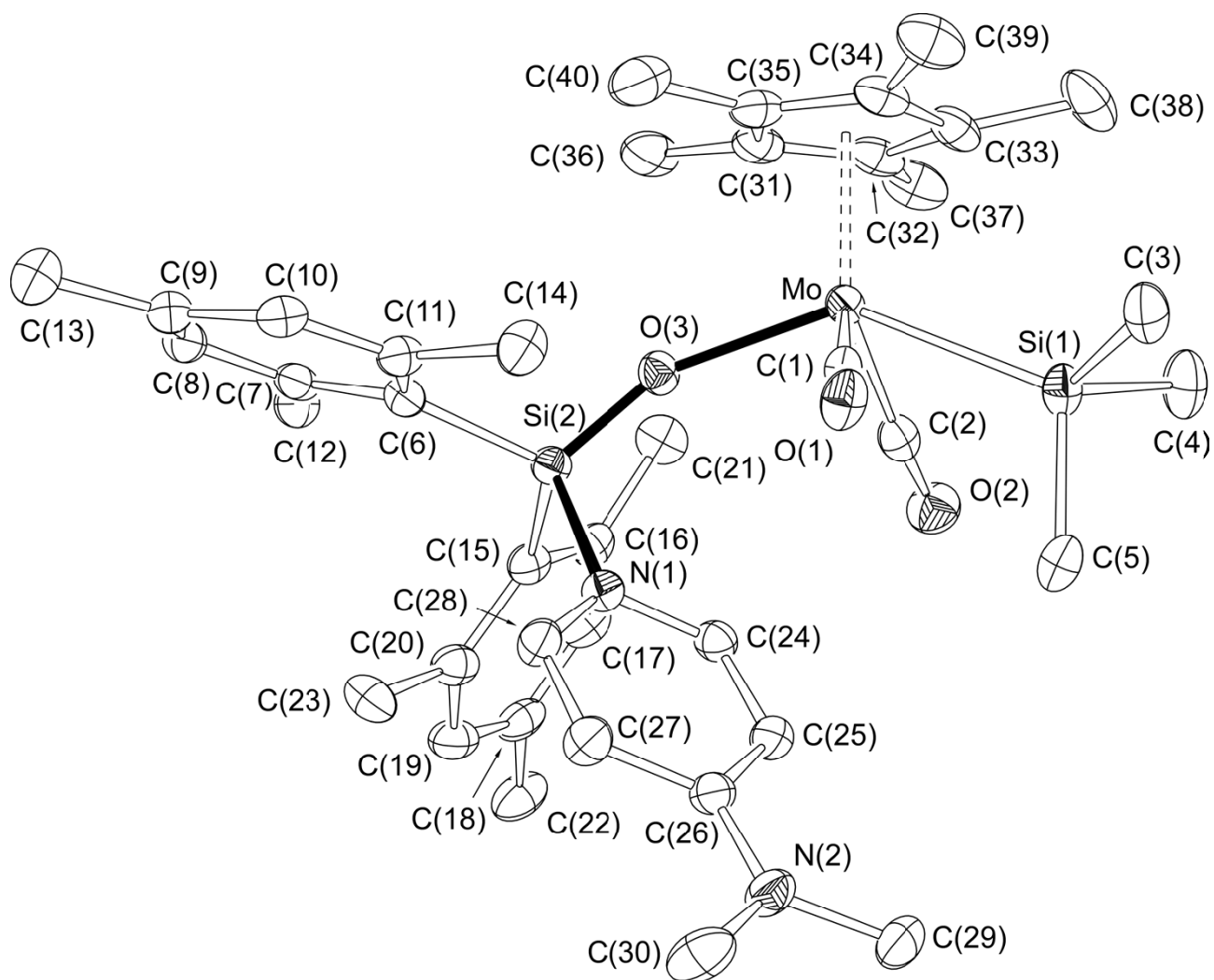


Figure S-1. ORTEP drawing of **2a** (thermal ellipsoids at the 50% probability level).

Table S-5. Crystal data and structure refinement for complex **2b**·toluene.

Complex	Cp*(OC) ₂ Mo(SiMe ₃){O=SiMe ₂ (PNO)}·C ₇ H ₈ (2b ·toluene)	
Empirical formula	C ₄₅ H ₅₉ MoNO ₄ Si ₂	
Formula weight	830.05	
Temperature (K)	175(2)	
Wavelength (Å)	0.71073	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 11.73(2) Å	α = 99.65(9)°
	<i>b</i> = 11.98(3) Å	β = 91.68(8)°
	<i>c</i> = 15.85(6) Å	γ = 97.94(9)°
Volume (Å ³)	2172(11)	
<i>Z</i>	2	
<i>D</i> _{calc} (Mg / m ³)	1.269	
Absorption coefficient (mm ⁻¹)	0.398	
<i>F</i> (000)	876	
Crystal Size (mm ³)	0.2 × 0.2 × 0.05	
θ Range for data collection (°)	1.31 – 25.00	
Index ranges	−12 ≤ <i>h</i> ≤ 13, −14 ≤ <i>k</i> ≤ 14, −18 ≤ <i>l</i> ≤ 18	
Reflections collected	19447	
Independent reflections [<i>R</i> (int)]	7181 [0.1889]	
Absorption correction	Semi-empirical from equivalents	
Maximum and minimum transmission	1.000 and 0.6778	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	7181 / 250 / 533	
Goodness-of-fit on <i>F</i> ²	1.176	
Final <i>R</i> indices ^a [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.1162, <i>wR</i> 2 = 0.3162	
<i>R</i> indices ^a (all data)	<i>R</i> 1 = 0.1302, <i>wR</i> 2 = 0.3296	
Largest difference in peak and hole (eÅ ⁻³)	2.803 and -0.515	

^a*R*1 = $\Sigma||F_o| - |F_c|| / \Sigma|F_o|$.

*wR*2 = $[\Sigma[w (F_o^2 - F_c^2)^2] / \Sigma[w (F_o^2)^2]]^{0.5}$,

calc *w* = 1 / [$\sigma^2(F_o^2) + (0.1380 P)^2 + 4.6356 P$] where *P* = (*F*_o² + 2*F*_c²) / 3.

Table S-6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2b**·toluene. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Mo	5392(1)	2648(1)	7731(1)	58(1)
Si(1)	4450(3)	3124(3)	6335(2)	90(1)
Si(2)	7951(2)	1349(2)	8000(2)	56(1)
O(1)	7245(8)	3917(9)	6736(7)	118(3)
O(2)	4071(8)	496(7)	6550(5)	107(3)
O(3)	6711(5)	1654(5)	8053(4)	59(1)
O(4)	8673(5)	2027(5)	7220(4)	64(2)
N	8499(7)	1605(7)	6396(5)	71(2)
C(1)	6544(9)	3375(10)	7065(8)	80(3)
C(2)	4638(10)	1312(9)	6944(6)	76(3)
C(3)	2835(11)	2578(12)	6109(8)	99(4)
C(4)	5119(17)	2448(18)	5324(8)	153(8)
C(5)	4648(13)	4708(14)	6275(10)	124(5)
C(6)	8927(7)	1914(7)	8974(5)	54(2)
C(7)	9656(6)	2992(6)	9108(5)	50(2)
C(8)	10410(7)	3289(7)	9840(6)	61(2)
C(9)	10435(8)	2621(8)	10463(6)	63(2)
C(10)	9668(8)	1621(8)	10345(6)	67(2)
C(11)	8922(8)	1276(7)	9643(6)	59(2)
C(12)	9687(8)	3829(7)	8506(6)	64(2)
C(13)	11286(11)	2959(10)	11220(7)	91(3)
C(14)	8074(10)	181(8)	9602(7)	78(3)
C(15)	8102(7)	-188(7)	7538(5)	59(2)
C(16)	9171(8)	-511(8)	7324(5)	60(2)
C(17)	9217(9)	-1591(8)	6856(6)	67(2)
C(18)	8247(11)	-2381(8)	6596(6)	74(3)
C(19)	7225(10)	-2104(8)	6854(7)	75(3)
C(20)	7107(8)	-1057(8)	7346(7)	69(2)
C(21)	10283(8)	266(9)	7594(7)	73(3)
C(22)	8389(16)	-3557(10)	6079(9)	122(5)
C(23)	5923(10)	-917(10)	7651(10)	103(4)
C(24)	9385(11)	1735(11)	5925(7)	92(4)
C(25)	9288(13)	1244(14)	5076(8)	107(4)
C(26)	8250(13)	717(13)	4699(8)	106(4)

C(27)	7333(11)	627(11)	5199(7)	90(3)
C(28)	7445(9)	1069(9)	6065(6)	76(3)
C(29)	4916(10)	2591(10)	9165(7)	77(3)
C(30)	5686(9)	3628(11)	9147(7)	88(4)
C(31)	5095(9)	4300(9)	8684(7)	78(3)
C(32)	3990(8)	3674(9)	8409(6)	69(2)
C(33)	3919(9)	2636(9)	8722(7)	76(3)
C(34)	5182(16)	1659(15)	9601(9)	135(7)
C(35)	6875(12)	3953(18)	9590(9)	153(8)
C(36)	5470(14)	5532(11)	8557(11)	124(6)
C(37)	2999(12)	4146(14)	8092(9)	115(5)
C(38)	2836(11)	1741(13)	8620(10)	117(5)
C(51)	12244(16)	-2780(16)	7390(11)	107(5)
C(52)	11345(16)	-3582(18)	7559(9)	98(6)
C(53)	10826(14)	-4436(16)	6903(13)	106(6)
C(54)	11207(17)	-4497(17)	6077(11)	116(7)
C(55)	12107(19)	-3690(20)	5907(9)	110(6)
C(56)	12625(16)	-2832(18)	6564(13)	110(7)
C(57)	12840(30)	-1990(30)	7950(20)	124(12)
C(61)	12183(18)	-3426(17)	6514(11)	114(6)
C(62)	12869(19)	-2363(18)	6681(12)	112(7)
C(63)	12980(20)	-1730(16)	7506(14)	113(7)
C(64)	12410(20)	-2160(20)	8164(11)	116(8)
C(65)	11719(19)	-3220(20)	7997(12)	119(7)
C(66)	11608(17)	-3856(16)	7172(14)	111(6)
C(67)	12010(50)	-4170(40)	5810(30)	230(30)

Table S-7. Bond lengths [Å] and angles [°] for **2b**·toluene.

Mo-Si(1)	2.626(8)	C(17)-C(18)	1.380(15)
Mo-O(3)	2.176(7)	C(18)-C(19)	1.345(16)
Mo-C(1)	1.940(11)	C(18)-C(22)	1.539(15)
Mo-C(2)	1.942(11)	C(19)-C(20)	1.388(14)
Mo-C(29)	2.366(13)	C(20)-C(23)	1.505(16)
Mo-C(30)	2.344(12)	C(24)-C(25)	1.370(18)
Mo-C(31)	2.355(11)	C(25)-C(26)	1.36(2)
Mo-C(32)	2.366(10)	C(26)-C(27)	1.357(18)
Mo-C(33)	2.369(11)	C(27)-C(28)	1.381(15)
Si(1)-C(3)	1.918(14)	C(29)-C(30)	1.437(17)
Si(1)-C(4)	1.911(15)	C(29)-C(33)	1.358(15)
Si(1)-C(5)	1.899(17)	C(29)-C(34)	1.471(17)
Si(2)-O(3)	1.550(7)	C(30)-C(31)	1.410(18)
Si(2)-O(4)	1.764(7)	C(30)-C(35)	1.513(16)
Si(2)-C(6)	1.867(10)	C(31)-C(32)	1.422(14)
Si(2)-C(15)	1.899(10)	C(31)-C(36)	1.530(17)
O(1)-C(1)	1.166(12)	C(32)-C(33)	1.407(15)
O(2)-C(2)	1.175(12)	C(32)-C(37)	1.471(16)
O(4)-N	1.317(11)	C(33)-C(38)	1.531(14)
N-C(24)	1.305(13)	C(51)-C(52)	1.3900
N-C(28)	1.359(13)	C(51)-C(56)	1.3900
C(6)-C(7)	1.427(11)	C(51)-C(57)	1.29(3)
C(6)-C(11)	1.407(12)	C(52)-C(53)	1.3900
C(7)-C(8)	1.403(12)	C(53)-C(54)	1.3900
C(7)-C(12)	1.494(12)	C(54)-C(55)	1.3900
C(8)-C(9)	1.374(13)	C(55)-C(56)	1.3900
C(9)-C(10)	1.380(13)	C(61)-C(62)	1.3900
C(9)-C(13)	1.501(13)	C(61)-C(66)	1.3900
C(10)-C(11)	1.364(13)	C(61)-C(67)	1.30(3)
C(11)-C(14)	1.523(12)	C(62)-C(63)	1.3900
C(15)-C(16)	1.397(13)	C(63)-C(64)	1.3900
C(15)-C(20)	1.441(12)	C(64)-C(65)	1.3900
C(16)-C(17)	1.389(13)	C(65)-C(66)	1.3900
C(16)-C(21)	1.500(13)		
Si(1)-Mo-O(3)	137.25(18)	C(32)-Mo-C(33)	34.6(4)

Si(1)-Mo-C(1)	68.8(4)	Mo-Si(1)-C(3)	116.1(4)
Si(1)-Mo-C(2)	66.0(4)	Mo-Si(1)-C(4)	112.0(5)
Si(1)-Mo-C(29)	138.1(3)	Mo-Si(1)-C(5)	114.0(5)
Si(1)-Mo-C(30)	133.1(4)	C(3)-Si(1)-C(4)	103.1(8)
Si(1)-Mo-C(31)	98.2(4)	C(3)-Si(1)-C(5)	106.4(6)
Si(1)-Mo-C(32)	83.2(3)	C(4)-Si(1)-C(5)	103.9(8)
Si(1)-Mo-C(33)	105.4(4)	O(3)-Si(2)-O(4)	109.4(4)
O(3)-Mo-C(1)	86.1(4)	O(3)-Si(2)-C(6)	115.6(4)
O(3)-Mo-C(2)	89.3(4)	O(3)-Si(2)-C(15)	116.9(4)
O(3)-Mo-C(29)	82.6(3)	O(4)-Si(2)-C(6)	101.7(4)
O(3)-Mo-C(30)	86.3(4)	O(4)-Si(2)-C(15)	98.6(4)
O(3)-Mo-C(31)	119.7(4)	C(6)-Si(2)-C(15)	111.9(4)
O(3)-Mo-C(32)	139.4(4)	Mo-O(3)-Si(2)	151.2(4)
O(3)-Mo-C(33)	111.2(4)	Si(2)-O(4)-N	121.4(6)
C(1)-Mo-C(2)	104.6(6)	O(4)-N-C(24)	116.5(9)
C(1)-Mo-C(29)	141.3(5)	O(4)-N-C(28)	121.0(8)
C(1)-Mo-C(30)	107.1(5)	C(24)-N-C(28)	122.4(10)
C(1)-Mo-C(31)	97.6(5)	Mo-C(1)-O(1)	172.6(12)
C(1)-Mo-C(32)	120.8(4)	Mo-C(2)-O(2)	170.9(10)
C(1)-Mo-C(33)	154.2(4)	Si(2)-C(6)-C(7)	124.0(6)
C(2)-Mo-C(29)	112.1(5)	Si(2)-C(6)-C(11)	119.(6)
C(2)-Mo-C(30)	147.6(5)	C(7)-C(6)-C(11)	116.8(8)
C(2)-Mo-C(31)	144.7(4)	C(6)-C(7)-C(8)	118.8(8)
C(2)-Mo-C(32)	109.8(4)	C(6)-C(7)-C(12)	124.1(7)
C(2)-Mo-C(33)	94.9(4)	C(8)-C(7)-C(12)	117.1(7)
C(29)-Mo-C(30)	35.5(4)	C(7)-C(8)-C(9)	123.1(8)
C(29)-Mo-C(31)	58.0(4)	C(8)-C(9)-C(10)	116.8(8)
C(29)-Mo-C(32)	57.2(4)	C(8)-C(9)-C(13)	121.0(9)
C(29)-Mo-C(33)	33.3(4)	C(10)-C(9)-C(13)	122.2(9)
C(30)-Mo-C(31)	34.9(4)	C(9)-C(10)-C(11)	123.0(9)
C(30)-Mo-C(32)	58.2(4)	C(6)-C(11)-C(10)	121.2(8)
C(30)-Mo-C(33)	57.4(4)	C(6)-C(11)-C(14)	120.5(8)
C(31)-Mo-C(32)	35.1(3)	C(10)-C(11)-C(14)	118.3(8)
C(31)-Mo-C(33)	57.5(4)	Si(2)-C(15)-C(16)	121.6(6)
Si(2)-C(15)-C(20)	121.2(7)	Mo-C(31)-C(36)	125.4(8)
C(16)-C(15)-C(20)	117.1(8)	C(30)-C(31)-C(32)	107.9(10)
C(15)-C(16)-C(17)	119.5(9)	C(30)-C(31)-C(36)	128.3(12)
C(15)-C(16)-C(21)	122.2(8)	C(32)-C(31)-C(36)	123.5(12)

C(17)-C(16)-C(21)	118.3(9)	Mo-C(32)-C(31)	72.1(6)
C(16)-C(17)-C(18)	122.9(10)	Mo-C(32)-C(33)	72.8(6)
C(17)-C(18)-C(19)	117.9(9)	Mo-C(32)-C(37)	133.7(8)
C(17)-C(18)-C(22)	119.0(12)	C(31)-C(32)-C(33)	106.9(9)
C(19)-C(18)-C(22)	123.1(12)	C(31)-C(32)-C(37)	125.9(11)
C(18)-C(19)-C(20)	122.9(10)	C(33)-C(32)-C(37)	125.0(11)
C(15)-C(20)-C(19)	119.2(10)	Mo-C(33)-C(29)	73.2(6)
C(15)-C(20)-C(23)	124.3(10)	Mo-C(33)-C(32)	72.6(5)
C(19)-C(20)-C(23)	116.5(9)	Mo-C(33)-C(38)	124.0(7)
N-C(24)-C(25)	119.6(12)	C(29)-C(33)-C(32)	110.0(9)
C(24)-C(25)-C(26)	120.7(13)	C(29)-C(33)-C(38)	125.9(12)
C(25)-C(26)-C(27)	118.3(12)	C(32)-C(33)-C(38)	123.9(12)
C(26)-C(27)-C(28)	121.0(11)	C(52)-C(51)-C(56)	120.0
N-C(28)-C(27)	117.8(10)	C(52)-C(51)-C(57)	126.0(19)
Mo-C(29)-C(30)	71.4(6)	C(56)-C(51)-C(57)	113.9(19)
Mo-C(29)-C(33)	73.4(6)	C(51)-C(52)-C(53)	120.0
Mo-C(29)-C(34)	121.4(8)	C(52)-C(53)-C(54)	120.0
C(30)-C(29)-C(33)	108.2(10)	C(53)-C(54)-C(55)	120.0
C(30)-C(29)-C(34)	124.9(13)	C(54)-C(55)-C(56)	120.0
C(33)-C(29)-C(34)	126.9(13)	C(51)-C(56)-C(55)	120.0
Mo-C(30)-C(29)	73.1(6)	C(62)-C(61)-C(66)	120.0
Mo-C(30)-C(31)	72.9(6)	C(62)-C(61)-C(67)	130(2)
Mo-C(30)-C(35)	122.1(8)	C(66)-C(61)-C(67)	110(2)
C(29)-C(30)-C(31)	106.9(10)	C(61)-C(62)-C(63)	120.0
C(29)-C(30)-C(35)	125.8(14)	C(62)-C(63)-C(64)	120.0
C(31)-C(30)-C(35)	127.2(14)	C(63)-C(64)-C(65)	120.0
Mo-C(31)-C(30)	72.1(6)	C(64)-C(65)-C(66)	120.0
Mo-C(31)-C(32)	72.9(6)	C(61)-C(66)-C(65)	120.0

Table S-8. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2b**-toluene. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo	49(1)	71(1)	52(1)	3(1)	2(1)	10(1)

Si(1)	81(2)	122(3)	78(2)	35(2)	5(2)	33(2)
Si(2)	44(1)	60(1)	58(1)	2(1)	2(1)	2(1)
O(1)	88(6)	128(7)	162(9)	82(7)	46(6)	22(5)
O(2)	122(7)	102(6)	81(5)	-10(4)	-46(5)	9(5)
O(3)	46(3)	73(4)	57(3)	4(3)	0(2)	12(3)
O(4)	61(4)	75(4)	49(3)	1(3)	6(3)	-4(3)
N	63(5)	75(5)	69(5)	-1(4)	2(4)	7(4)
C(1)	57(6)	91(7)	109(8)	46(6)	31(5)	27(5)
C(2)	81(7)	87(7)	54(5)	-8(5)	-12(5)	19(5)
C(3)	102(10)	131(10)	68(7)	19(7)	-18(6)	30(7)
C(4)	191(18)	240(20)	60(7)	60(10)	43(9)	107(15)
C(5)	107(11)	169(15)	124(12)	79(11)	14(9)	50(10)
C(6)	45(5)	62(5)	52(4)	3(4)	8(3)	9(3)
C(7)	37(4)	47(4)	61(5)	1(3)	4(3)	4(3)
C(8)	46(5)	62(5)	67(5)	2(4)	4(4)	-5(4)
C(9)	60(6)	67(5)	59(5)	10(4)	-7(4)	6(4)
C(10)	70(6)	70(6)	60(5)	19(4)	10(4)	-5(4)
C(11)	55(5)	58(5)	61(5)	10(4)	8(4)	-1(4)
C(12)	61(6)	61(5)	65(5)	7(4)	-9(4)	-2(4)
C(13)	95(8)	91(8)	76(7)	12(6)	-29(6)	-13(6)
C(14)	92(8)	62(5)	76(6)	16(5)	21(5)	-10(5)
C(15)	51(5)	63(5)	56(5)	-2(4)	-9(4)	3(4)
C(16)	51(5)	76(6)	53(5)	12(4)	1(3)	11(4)
C(17)	85(7)	70(6)	55(5)	19(4)	22(4)	26(5)
C(18)	117(9)	54(5)	49(5)	4(4)	-5(5)	13(5)
C(19)	83(7)	58(5)	76(6)	2(5)	-18(5)	0(5)
C(20)	56(6)	65(5)	83(6)	6(5)	-13(4)	9(4)
C(21)	51(6)	86(7)	85(7)	21(5)	18(5)	16(4)
C(22)	206(17)	62(7)	94(9)	-6(6)	7(10)	23(8)
C(23)	59(7)	80(7)	154(12)	-9(7)	-18(7)	-4(5)
C(24)	96(8)	122(9)	53(6)	21(6)	22(5)	-12(7)
C(25)	95(10)	151(13)	77(8)	18(8)	22(7)	20(8)
C(26)	116(12)	139(12)	65(7)	4(7)	1(7)	47(9)
C(27)	85(8)	115(9)	59(6)	-18(6)	-11(5)	20(6)
C(28)	66(6)	93(7)	65(6)	2(5)	-4(5)	14(5)
C(29)	81(8)	93(7)	62(6)	14(5)	15(5)	31(6)
C(30)	55(6)	123(9)	69(6)	-37(6)	0(5)	17(6)
C(31)	60(6)	75(6)	92(7)	-4(5)	22(5)	3(5)

C(32)	49(5)	84(7)	70(6)	-5(5)	8(4)	16(4)
C(33)	64(7)	78(7)	76(6)	-8(5)	20(5)	3(5)
C(34)	173(17)	182(16)	85(9)	49(10)	46(10)	101(13)
C(35)	76(10)	260(20)	93(10)	-55(11)	-29(7)	31(11)
C(36)	130(12)	76(8)	157(14)	-1(8)	49(10)	-3(8)
C(37)	88(10)	152(13)	106(10)	-5(9)	-5(7)	53(8)
C(38)	80(9)	129(11)	123(11)	-4(8)	42(8)	-32(8)
C(51)	81(11)	147(14)	106(10)	35(10)	12(9)	47(9)
C(52)	92(13)	148(15)	80(11)	60(10)	26(10)	58(10)
C(53)	88(14)	135(15)	118(13)	60(11)	13(10)	45(10)
C(54)	87(14)	152(17)	115(12)	20(12)	14(11)	41(11)
C(55)	86(14)	157(18)	107(12)	39(11)	39(12)	61(11)
C(56)	73(13)	150(16)	123(12)	50(11)	34(10)	32(11)
C(57)	61(18)	200(30)	110(20)	23(17)	33(15)	12(17)
C(61)	88(13)	150(15)	117(11)	31(11)	25(11)	47(11)
C(62)	85(14)	154(16)	111(11)	43(12)	31(12)	38(11)
C(63)	86(15)	146(16)	120(14)	39(11)	30(13)	36(11)
C(64)	94(19)	162(17)	107(13)	29(13)	38(13)	51(12)
C(65)	109(17)	157(16)	117(12)	69(12)	23(13)	46(12)
C(66)	83(13)	139(14)	129(13)	56(10)	10(11)	37(11)
C(67)	180(40)	160(40)	300(40)	-100(30)	50(40)	10(30)

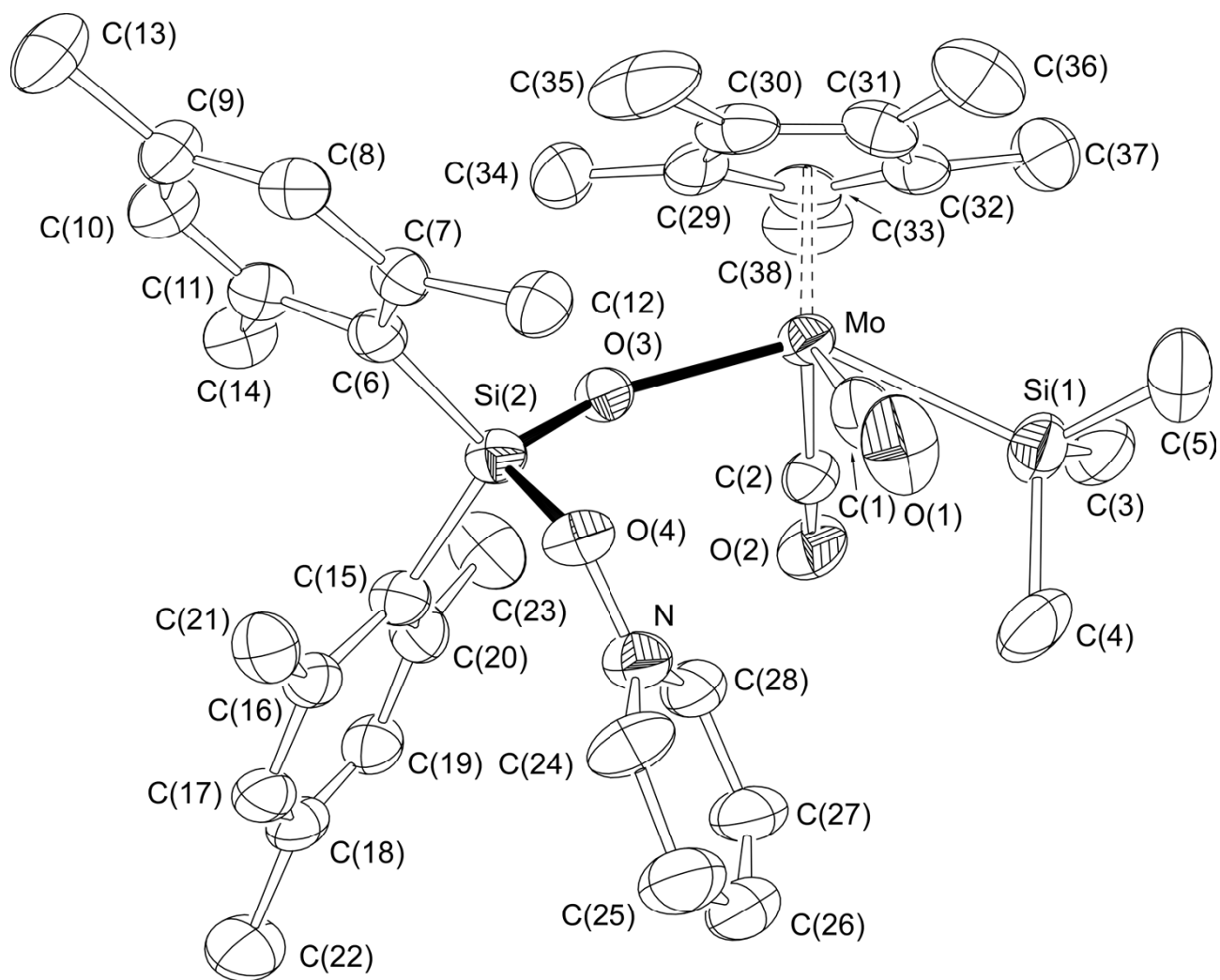


Figure S-2. ORTEP drawing of **2b** (thermal ellipsoids at the 50% probability level).

Table S-9. Crystal data and structure refinement for complex **3**.

Complex	Cp*(OC) ₂ Mo(SiMe ₃)(DMAP) (3)	
Empirical formula	C ₂₂ H ₃₄ MoN ₂ O ₂ Si	
Formula weight	482.54	
Temperature (K)	150(2)	
Wavelength (Å)	0.71073	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	<i>a</i> = 8.8649(10) Å	<i>α</i> = 100.209(2) °
	<i>b</i> = 9.3915(10) Å	<i>β</i> = 96.929(2) °
	<i>c</i> = 15.3505(15) Å	<i>γ</i> = 110.704(3) °
Volume (Å ³)	1153.0(2)	
<i>Z</i>	2	
<i>D</i> _{calc} (Mg / m ³)	1.390	
Absorption coefficient (mm ⁻¹)	0.640	
<i>F</i> (000)	504	
Crystal Size (mm ³)	0.25 × 0.20 × 0.15	
<i>θ</i> Range for data collection (°)	1.38 – 27.50	
Index ranges	–11 ≤ <i>h</i> ≤ 11, –12 ≤ <i>k</i> ≤ 12, –19 ≤ <i>l</i> ≤ 19	
Reflections collected	10633	
Independent reflections [<i>R</i> (int)]	4888 [0.0254]	
Absorption correction	Semi-empirical from equivalents	
Maximum and minimum transmission	1.000 and 0.8470	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	4888 / 192 / 359	
Goodness-of-fit on <i>F</i> ²	1.152	
Final <i>R</i> indices ^a [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0284, <i>wR</i> 2 = 0.0743	
<i>R</i> indices ^a (all data)	<i>R</i> 1 = 0.0287, <i>wR</i> 2 = 0.0745	
Largest difference in peak and hole (eÅ ⁻³)	0.527 and -0.680	

^a*R*1 = Σ||*F**o*| - |*F**c*|| / Σ|*F**o*|.

*wR*2 = [Σ[*w* (*F**o*² - *F**c*²)²] / Σ[*w* (*F**o*²)²]]^{0.5},

calc *w* = 1 / [σ²(*F**o*²) + (0.0302 *P*)² + 0.7403 *P*] where *P* = (*F**o*² + 2*F**c*²) / 3.

Table S-10. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Mo	56(1)	3416(1)	2311(1)	17(1)
Si	-2548(1)	907(1)	2212(1)	23(1)
O(1)	1000(3)	509(3)	2136(2)	55(1)
O(2)	-1574(2)	3713(2)	3982(1)	39(1)
N(1)	2402(2)	4707(2)	3331(1)	20(1)
N(2)	6962(2)	7622(2)	5023(1)	30(1)
C(1)	635(3)	1582(3)	2250(2)	28(1)
C(2)	-956(3)	3555(3)	3361(2)	24(1)
C(3)	-2373(4)	-87(3)	3174(2)	44(1)
C(4)	-3066(3)	-735(3)	1178(2)	39(1)
C(5)	-4527(3)	1246(3)	2253(2)	40(1)
C(6)	3804(3)	4467(2)	3253(2)	23(1)
C(7)	5319(3)	5374(3)	3793(1)	25(1)
C(8)	5500(3)	6669(2)	4484(1)	23(1)
C(9)	4029(3)	6891(3)	4586(1)	27(1)
C(10)	2570(3)	5910(3)	4018(2)	25(1)
C(11)	8474(3)	7408(3)	4890(2)	35(1)
C(12)	7112(3)	9028(3)	5663(2)	43(1)
C(13)	-1431(6)	3786(9)	1035(5)	45(2)
C(14)	-609(8)	5282(6)	1640(4)	40(1)
C(15)	1101(6)	5668(5)	1694(4)	33(1)
C(16)	1339(6)	4407(7)	1145(3)	36(1)
C(17)	-224(8)	3241(6)	727(3)	47(2)
C(18)	-3234(6)	3042(9)	600(5)	92(3)
C(19)	-1403(8)	6318(7)	2063(5)	80(2)
C(20)	2439(6)	7213(5)	2185(3)	55(1)
C(21)	2962(6)	4380(7)	947(3)	61(1)
C(22)	-498(8)	1820(7)	-18(3)	91(2)
C(33)	-1328(11)	4657(13)	1543(6)	27(2)
C(34)	251(13)	5767(7)	1965(4)	17(1)
C(35)	1411(10)	5258(11)	1580(7)	19(2)
C(36)	542(16)	3844(11)	934(5)	19(2)
C(37)	-1139(16)	3437(12)	914(8)	22(2)
C(38)	-2892(12)	4917(15)	1650(8)	57(3)

C(39)	685(16)	7349(9)	2605(5)	50(3)
C(40)	3251(9)	6201(12)	1766(7)	47(2)
C(41)	1303(15)	2967(11)	321(6)	49(3)
C(42)	-2427(17)	2164(12)	166(7)	67(4)

Table S-11. Bond lengths [Å] and angles [°] for **3**.

Mo-Si	2.6169(6)	C(6)-C(7)	1.375(3)
Mo-N(1)	2.2377(17)	C(7)-C(8)	1.412(3)
Mo-C(1)	1.953(2)	C(8)-C(9)	1.413(3)
Mo-C(2)	1.944(2)	C(9)-C(10)	1.373(3)
Mo-C(13)	2.374(6)	C(13)-C(14)	1.420(7)
Mo-C(14)	2.389(4)	C(13)-C(17)	1.433(8)
Mo-C(15)	2.401(5)	C(13)-C(18)	1.508(5)
Mo-C(16)	2.387(4)	C(14)-C(15)	1.417(7)
Mo-C(17)	2.384(4)	C(14)-C(19)	1.494(5)
Mo-C(33)	2.324(8)	C(15)-C(16)	1.423(6)
Mo-C(34)	2.315(6)	C(15)-C(20)	1.503(5)
Mo-C(35)	2.289(10)	C(16)-C(17)	1.412(6)
Mo-C(36)	2.283(6)	C(16)-C(21)	1.514(5)
Mo-C(37)	2.280(12)	C(17)-C(22)	1.520(6)
Si-C(3)	1.899(3)	C(33)-C(34)	1.406(10)
Si-C(4)	1.888(3)	C(33)-C(37)	1.434(13)
Si-C(5)	1.897(3)	C(33)-C(38)	1.513(7)
O(1)-C(1)	1.155(3)	C(34)-C(35)	1.425(10)
O(2)-C(2)	1.167(3)	C(34)-C(39)	1.520(7)
N(1)-C(6)	1.356(3)	C(35)-C(36)	1.403(10)
N(1)-C(10)	1.354(3)	C(35)-C(40)	1.518(8)
N(2)-C(8)	1.351(3)	C(36)-C(37)	1.396(17)
N(2)-C(11)	1.456(3)	C(36)-C(41)	1.513(10)
N(2)-C(12)	1.453(3)	C(37)-C(42)	1.512(8)
Si-Mo-N(1)	133.26(5)	Si-Mo-C(34)	129.9(2)
Si-Mo-C(1)	69.30(8)	Si-Mo-C(35)	146.3(3)
Si-Mo-C(2)	66.99(7)	Si-Mo-C(36)	113.6(3)
Si-Mo-C(13)	87.0(2)	Si-Mo-C(37)	86.7(3)
Si-Mo-C(14)	112.1(2)	N(1)-Mo-C(1)	86.03(8)
Si-Mo-C(15)	143.8(1)	N(1)-Mo-C(2)	83.56(8)
Si-Mo-C(16)	130.3(1)	N(1)-Mo-C(13)	139.1(2)
Si-Mo-C(17)	96.6(1)	N(1)-Mo-C(14)	107.9(2)
Si-Mo-C(33)	95.8(3)	N(1)-Mo-C(15)	82.1(1)
N(1)-Mo-C(16)	91.3(1)	C(14)-Mo-C(15)	34.4(2)
N(1)-Mo-C(17)	125.2(2)	C(14)-Mo-C(16)	57.9(2)

N(1)-Mo-C(33)	123.3(3)	C(14)-Mo-C(17)	58.1(2)
N(1)-Mo-C(34)	88.8(2)	C(14)-Mo-C(33)	16.4(3)
N(1)-Mo-C(35)	80.2(2)	C(14)-Mo-C(34)	19.2(3)
N(1)-Mo-C(36)	108.4(3)	C(14)-Mo-C(35)	45.5(3)
N(1)-Mo-C(37)	139.9(3)	C(14)-Mo-C(36)	55.6(3)
C(1)-Mo-C(2)	105.64(9)	C(15)-Mo-C(16)	34.6(2)
C(1)-Mo-C(13)	121.8(2)	C(15)-Mo-C(17)	57.3(2)
C(1)-Mo-C(14)	152.25(14)	C(15)-Mo-C(33)	49.7(3)
C(1)-Mo-C(15)	131.1(2)	C(15)-Mo-C(34)	22.6(2)
C(1)-Mo-C(16)	99.1(2)	C(15)-Mo-C(35)	13.5(3)
C(1)-Mo-C(17)	94.2(2)	C(15)-Mo-C(36)	44.0(3)
C(1)-Mo-C(33)	146.0(3)	C(15)-Mo-C(37)	59.2(3)
C(1)-Mo-C(34)	153.6(2)	C(16)-Mo-C(17)	34.4(2)
C(1)-Mo-C(35)	117.6(3)	C(16)-Mo-C(33)	66.7(3)
C(1)-Mo-C(36)	97.6(2)	C(16)-Mo-C(34)	55.2(2)
C(1)-Mo-C(37)	110.5(3)	C(16)-Mo-C(35)	22.7(3)
C(2)-Mo-C(13)	112.5(2)	C(16)-Mo-C(36)	17.3(3)
C(2)-Mo-C(14)	99.81(13)	C(16)-Mo-C(37)	51.1(3)
C(2)-Mo-C(15)	119.8(1)	C(17)-Mo-C(33)	56.2(3)
C(2)-Mo-C(16)	154.3(2)	C(17)-Mo-C(34)	68.1(2)
C(2)-Mo-C(17)	146.6(2)	C(17)-Mo-C(35)	51.5(3)
C(2)-Mo-C(33)	95.2(2)	C(17)-Mo-C(36)	17.2(3)
C(2)-Mo-C(34)	99.4(2)	C(17)-Mo-C(37)	23.6(3)
C(2)-Mo-C(35)	132.2(3)	C(33)-Mo-C(34)	35.3(3)
C(2)-Mo-C(36)	154.7(2)	C(33)-Mo-C(35)	59.3(3)
C(2)-Mo-C(37)	123.2(4)	C(33)-Mo-C(36)	59.5(3)
C(13)-Mo-C(14)	34.7(2)	C(33)-Mo-C(37)	36.3(3)
C(13)-Mo-C(15)	57.0(2)	C(34)-Mo-C(35)	36.1(3)
C(13)-Mo-C(16)	57.6(2)	C(34)-Mo-C(36)	59.8(2)
C(13)-Mo-C(17)	35.1(2)	C(34)-Mo-C(37)	60.0(3)
C(13)-Mo-C(33)	24.4(3)	C(35)-Mo-C(36)	35.7(3)
C(13)-Mo-C(34)	52.5(3)	C(35)-Mo-C(37)	59.7(4)
C(13)-Mo-C(35)	60.8(3)	C(36)-Mo-C(37)	35.6(4)
C(13)-Mo-C(36)	44.3(3)	Mo-Si-C(3)	113.62(8)
Mo-Si-C(4)	115.63(9)	C(14)-C(15)-C(20)	125.5(5)
Mo-Si-C(5)	115.13(9)	C(16)-C(15)-C(20)	125.4(5)
C(3)-Si-C(4)	102.71(13)	Mo-C(16)-C(15)	73.3(3)
C(3)-Si-C(5)	103.43(13)	Mo-C(16)-C(17)	72.7(2)

C(4)-Si-C(5)	104.79(12)	Mo-C(16)-C(21)	125.3(3)
Mo-N(1)-C(6)	122.75(13)	C(15)-C(16)-C(17)	108.1(4)
Mo-N(1)-C(10)	121.96(13)	C(15)-C(16)-C(21)	126.5(5)
C(6)-N(1)-C(10)	114.9(2)	C(17)-C(16)-C(21)	125.1(6)
C(8)-N(2)-C(11)	121.1(2)	Mo-C(17)-C(13)	72.1(3)
C(8)-N(2)-C(12)	120.7(2)	Mo-C(17)-C(16)	72.9(2)
C(11)-N(2)-C(12)	117.5(2)	Mo-C(17)-C(22)	127.6(4)
Mo-C(1)-O(1)	173.8(2)	C(13)-C(17)-C(16)	107.3(5)
Mo-C(2)-O(2)	176.3(2)	C(13)-C(17)-C(22)	128.1(6)
N(1)-C(6)-C(7)	124.6(2)	C(16)-C(17)-C(22)	123.9(6)
C(6)-C(7)-C(8)	120.3(2)	Mo-C(33)-C(34)	72.4(4)
N(2)-C(8)-C(7)	122.9(2)	Mo-C(33)-C(37)	70.2(6)
N(2)-C(8)-C(9)	121.8(2)	Mo-C(33)-C(38)	131.2(6)
C(7)-C(8)-C(9)	115.2(2)	C(34)-C(33)-C(37)	107.9(7)
C(8)-C(9)-C(10)	120.1(2)	C(34)-C(33)-C(38)	123.3(10)
N(1)-C(10)-C(9)	124.8(2)	C(37)-C(33)-C(38)	128.1(11)
Mo-C(13)-C(14)	73.2(3)	Mo-C(34)-C(33)	72.7(4)
Mo-C(13)-C(17)	72.9(3)	Mo-C(34)-C(35)	71.0(5)
Mo-C(13)-C(18)	131.2(4)	Mo-C(34)-C(39)	128.5(5)
C(14)-C(13)-C(17)	108.7(4)	C(33)-C(34)-C(35)	107.4(5)
C(14)-C(13)-C(18)	126.5(7)	C(33)-C(34)-C(39)	127.5(10)
C(17)-C(13)-C(18)	123.2(7)	C(35)-C(34)-C(39)	124.5(9)
Mo-C(14)-C(13)	72.1(3)	Mo-C(35)-C(34)	73.0(4)
Mo-C(14)-C(15)	73.3(2)	Mo-C(35)-C(36)	71.9(5)
Mo-C(14)-C(19)	124.6(3)	Mo-C(35)-C(40)	126.5(6)
C(13)-C(14)-C(15)	107.0(4)	C(34)-C(35)-C(36)	108.3(6)
C(13)-C(14)-C(19)	126.3(6)	C(34)-C(35)-C(40)	124.9(9)
C(15)-C(14)-C(19)	126.5(6)	C(36)-C(35)-C(40)	126.4(11)
Mo-C(15)-C(14)	72.3(2)	Mo-C(36)-C(35)	72.3(5)
Mo-C(15)-C(16)	72.2(3)	Mo-C(36)-C(37)	72.1(6)
Mo-C(15)-C(20)	125.6(3)	Mo-C(36)-C(41)	124.5(5)
C(14)-C(15)-C(16)	108.9(4)	C(35)-C(36)-C(37)	108.6(6)
C(35)-C(36)-C(41)	125.3(12)	Mo-C(37)-C(42)	132.2(8)
C(37)-C(36)-C(41)	125.9(11)	C(33)-C(37)-C(36)	107.7(8)
Mo-C(37)-C(33)	73.5(6)	C(33)-C(37)-C(42)	128.3(13)
Mo-C(37)-C(36)	72.3(5)	C(36)-C(37)-C(42)	121.9(12)

Table S-12. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*U_{11} + \dots + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo	15(1)	14(1)	20(1)	4(1)	0(1)	3(1)
Si	17(1)	17(1)	30(1)	7(1)	0(1)	3(1)
O(1)	38(1)	28(1)	89(2)	-10(1)	-15(1)	21(1)
O(2)	37(1)	48(1)	31(1)	3(1)	14(1)	15(1)
N(1)	16(1)	17(1)	23(1)	3(1)	0(1)	5(1)
N(2)	21(1)	32(1)	25(1)	1(1)	-4(1)	3(1)
C(1)	17(1)	23(1)	38(1)	-1(1)	-4(1)	6(1)
C(2)	19(1)	19(1)	29(1)	4(1)	-1(1)	6(1)
C(3)	38(2)	30(1)	52(2)	24(1)	-7(1)	-4(1)
C(4)	28(1)	23(1)	51(2)	-4(1)	-9(1)	2(1)
C(5)	20(1)	47(2)	53(2)	14(1)	9(1)	10(1)
C(6)	19(1)	19(1)	28(1)	1(1)	-1(1)	6(1)
C(7)	19(1)	24(1)	30(1)	5(1)	0(1)	8(1)
C(8)	18(1)	23(1)	20(1)	5(1)	-1(1)	2(1)
C(9)	25(1)	25(1)	24(1)	-4(1)	2(1)	6(1)
C(10)	21(1)	25(1)	26(1)	1(1)	2(1)	9(1)
C(11)	21(1)	35(1)	39(1)	5(1)	-6(1)	5(1)
C(12)	31(2)	43(2)	33(1)	-11(1)	-4(1)	1(1)
C(13)	21(2)	41(4)	44(3)	40(3)	-8(2)	-2(2)
C(14)	28(3)	46(3)	60(3)	41(2)	7(2)	16(2)
C(15)	26(2)	31(2)	39(3)	26(2)	1(2)	1(2)
C(16)	29(2)	51(3)	26(2)	22(2)	9(2)	3(2)
C(17)	41(3)	60(3)	19(2)	15(2)	1(2)	-6(2)
C(18)	31(3)	123(5)	100(4)	90(4)	-26(2)	-13(3)
C(19)	83(4)	78(4)	133(5)	75(4)	50(4)	62(4)
C(20)	51(3)	32(2)	67(3)	30(2)	-4(2)	-7(2)
C(21)	50(3)	90(4)	50(2)	33(3)	30(2)	21(3)
C(22)	92(5)	109(5)	21(2)	-10(2)	18(2)	-10(3)
C(33)	26(4)	37(4)	29(3)	23(3)	9(3)	17(3)
C(34)	31(4)	14(3)	15(3)	10(2)	10(3)	13(3)
C(35)	18(4)	20(4)	21(3)	13(3)	8(3)	5(3)
C(36)	31(5)	16(3)	14(3)	7(3)	11(3)	9(3)
C(37)	34(5)	12(3)	14(3)	9(2)	-4(3)	1(3)
C(38)	42(5)	92(7)	83(7)	69(6)	33(5)	51(5)

C(39)	111(8)	20(3)	31(4)	10(3)	16(4)	35(4)
C(40)	24(4)	56(5)	59(5)	39(4)	11(3)	1(4)
C(41)	97(7)	40(5)	39(4)	21(4)	39(5)	47(5)
C(42)	72(8)	45(5)	42(5)	26(4)	-33(5)	-21(5)

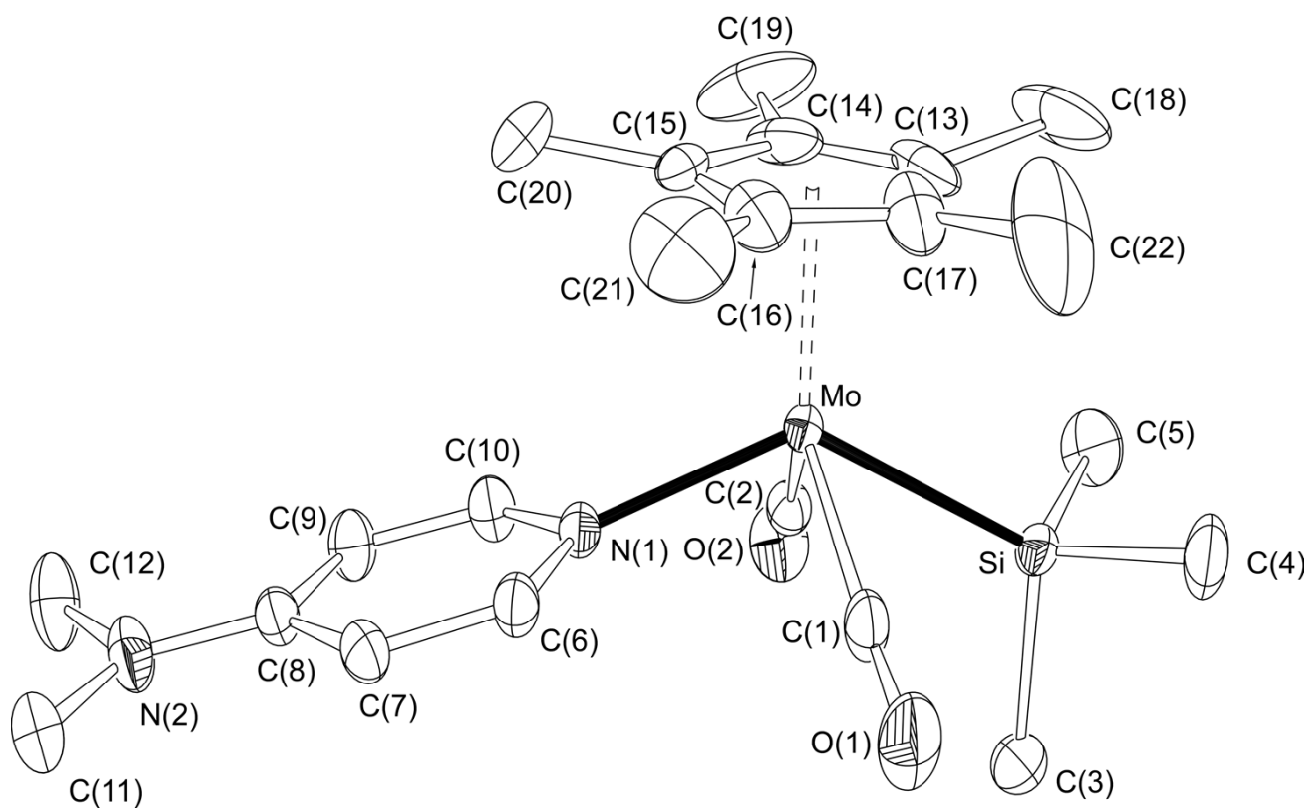


Figure S-3. ORTEP drawing of **3** (thermal ellipsoids at the 50% probability level).

4. References

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